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A hierarchical, spherical harmonic-based approach to simulate abradable, irregularly shaped particles in DEM

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Abstract

A novel approach is presented for simulating non-spherical particles in the discrete element method (DEM). A particle's shape is described through a hierarchy of representations using spherical harmonic expansions. The expansion is computed at nodes, obtained by discretising the particle's surface. A low-degree expansion, i.e., one containing few terms, is sufficient to approximate a particle's overall shape without any surface texture. Expansions are computed to high degrees only at interparticle contacts, rather than for the entire particle, which reduces the computational cost. The advantages of this approach include the ability to simulate a wide range of particle shapes and adaptive resolution depending on spatial and temporal considerations. An additional unique benefit is that changes of particle shape due to chipping can be captured in DEM for the first time. This is accomplished by progressively omitting more of the highest-degree terms from the expansion to give an increasingly smooth surface.

Keywords: Discrete element method (DEM), Adaptive resolution, Contact

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1. Introduction

Particle shape plays a fundamental role in the statics, dynamics and resistance to attrition of granular materials. It affects the height and porosity of a static bed of particles [1]. Particle shape affects the angle of repose in both a quasi-static sandpile [2, 3] and a rotating drum [4, 5]. In dynamic systems, variability in particle shape can induce segregation [6, 7] or affect flow rates [8, 9], mechanical behaviour [10, 11] or the particles' wearing propensity [12–14].

Despite the recognised importance of particle shape, spheres have often been used to represent particles in discrete element method (DEM) simulations, irrespective of their real shapes. Spheres have the great advantage of computational simplicity: straightforward contact detection, orientation independence and low memory requirements. However, spheres are often inadequate if quantitative agreement with a real, physical system is sought. Increasing computational resources have encouraged a commensurate increase in research activity in the modelling of granular systems composed of non-spherical particles in recent years [15–17].

The simplest option, though often inadequate [18, 19], is to combine spheres with a rotational resistance model which imposes torque terms at each interparticle contact to inhibit rolling and twisting motions. Replacing spheres with ellipsoids [20] or superquadrics [21] – a generalisation of ellipsoids – introduces non-sphericity but is limited to a subset of symmetrical shapes. Representing particles using polyhedra allows sharp edges and flat

24 surfaces to be simulated [22–24], but not in combination with curved surfaces.
 25 The aforementioned are ‘single-particle’ methods. However, the most com-
 26 mon approach to simulate non-spherical particles is the multi-sphere method:
 27 spheres are simply clumped together to create irregular clusters. This method
 28 is adopted in the commercial codes EDEM [25] and PFC [26]. Since spheres
 29 remain the fundamental particles, contact detection is simple [27]. However,
 30 many spheres may be required to obtain a reasonable approximation of a real
 31 particle’s shape [16, 28, 29]. Many less commonplace methods have also been
 32 proposed to capture non-spherical particle shapes in DEM, e.g., non-uniform
 33 rational B-splines [30], potential particles [31, 32] and spheropolyhedrons,
 34 generated from the Minkowski sum of a polyhedron with a sphere [33].

35 Some of these methods are restricted to a subset of particle shapes; others
 36 such as multi-spheres or polyhedra can, in principle, be used to simulate a
 37 particle of any arbitrary shape. Advances in X-ray computed tomographic
 38 imaging have enabled the measurement of particle morphology at a very
 39 high level of detail, equivalent to 15^3 – 25^3 voxels per sand grain [34]. It
 40 is unlikely that such a detailed representation, captured using a very large
 41 number of polyhedron faces or spheres in a multi-sphere cluster, is needed to
 42 simulate the behaviour of most granular systems adequately. Some studies
 43 have been done for specific situations, e.g., [35], but in general the fidelity
 44 of particle shape required to obtain an acceptable bulk response remains an
 45 open question.

46 One of the biggest challenges in modelling non-spherical particle shapes is
 47 contact detection. Two approaches are commonly used: continuous function
 48 representation (CFR) and discrete function representation (DFR). CFR uses

49 non-linear and iterative methods to detect and evaluate interparticle con-
 50 tacts, solving the equations which describe a particle’s shape [36]. In DFR
 51 [36–38], the surface of a particle is discretised into a set of surface nodes;
 52 contact detection involves evaluating whether any of these nodes lie inside
 53 a potentially contacting particle [27]. CFR and DFR can have comparable
 54 efficiency and accuracy on modern computing hardware [39]. Both are much
 55 more computationally expensive than contact detection for spheres. There-
 56 fore, a hierarchical representation of the geometry is often used to reduce
 57 the computational cost by cheaply eliminating a large proportion of non-
 58 contacts. Williams and O’Connor [38], for example, used four levels in their
 59 hierarchy: a bounding sphere, a bounding box, cellular regions and surface
 60 facets.

61 Another major challenge, one often ignored in DEM simulations, is changes
 62 of particle shape over time due to attrition, i.e., fragmentation or surface
 63 abrasion. Attrition is a particularly significant consideration for angular
 64 particles which are more susceptible to damage than rounded ones. The mo-
 65 tivation for considering attrition in simulations is its industrial importance.
 66 Fines reduce flowability which can impair processing operations such as con-
 67 veying, blending or tableting [40]. In the pharmaceutical sector, needle- and
 68 plate-type crystals are often produced [41]. Attrition of these crystals has
 69 major implications for product quality, affecting bulk density, specific sur-
 70 face area, segregation behaviour, dissolution rate and even surface chemistry
 71 [42, 43]. Attrition of infant formula disimproves the product’s rehydration
 72 characteristics and affects bulk density [44]. The mechanical degradation
 73 of catalysts, which necessitates their periodic replacement, is a significant

cost factor in fluidised bed processes [45]. Particle fragmentation can be simulated in two broad ways in DEM [46–48]: (i) agglomerates, created by joining the fundamental particles (usually spheres) with bonds of finite strengths, can disintegrate upon bond failure; (ii) particles are deemed to fail when a predefined force or stress is reached, after which they are replaced with smaller ‘daughter’ particles. However, there is no existing method to simulate abrading particles during a DEM simulation which takes into consideration the evolving particle shape. As an alternative, DEM simulations of non-abrading particles are sometimes performed to obtain data on the relevant particle dynamics, e.g., impact velocities, forces and collision frequencies, or estimated distributions of stresses and strains. These data are subsequently used as input to attrition models [42, 49].

In this paper, a novel approach is presented for modelling abradable, non-spherical particles in DEM which has several unique advantages:

- This approach is based on spherical harmonics, so inherently contains a hierarchical description of shape from a sphere to a highly refined representation with surface texture.
- Particles can be simulated with adaptive fidelity, e.g., depending on their location within the simulation domain or the time elapsed during the simulation.
- Abrasion can be captured by progressively omitting terms from the spherical harmonic expansion.

In addition, the approach is relatively straightforward to integrate into a sphere-based code. Section 2 describes how spherical harmonics can be used

to represent particle shapes. This is used and adapted in the novel DEM simulation approach described in Sections 3 and 4, which includes a demonstration of the method with two contacting particles. Section 5 demonstrates that the approach naturally includes the evolution of particle shape due to abrasion. Finally, some discussion of efficiency and the future implementation of the approach in a suitable code (such as LAMMPS [50]) is provided in Section 6.

2. Spherical harmonics for particle shape representation

We assume that the particle does not contain any voids and is ‘star-shaped’, i.e., any half-line drawn from a suitable origin, O , inside the particle crosses the particle’s contour exactly once. Therefore the particle can be analytically described by a function $r(\theta, \varphi)$ which is the distance from O . θ and φ are the polar angles, with $0 \leq \theta \leq \pi$ and $0 \leq \varphi \leq 2\pi$. The requirement for particles to be ‘star-shaped’ is rarely a limitation since a majority of natural particles fulfil this condition [51].

The function $r(\theta, \varphi)$ can be approximated as a truncated spherical harmonic series [51, 52] which is a generalisation to 3D of the Fourier series:

$$r(\theta, \varphi) \approx r_{SH}(N, \theta, \varphi) = \sum_{n=0}^N \sum_{m=-n}^n c_n^m Y_n^m(\theta, \varphi) \quad (1)$$

where $Y_n^m(\theta, \varphi)$ is the spherical harmonic function, n is the degree, m the order and N indicates the maximum degree at which the expansion is truncated. The function $Y_n^m(\theta, \varphi)$ is given by:

$$Y_n^m(\theta, \varphi) = \sqrt{\frac{(2n+1)(n-m)!}{4\pi(n+m)!}} P_n^m(\cos \theta) e^{im\varphi} \quad (2)$$

119 The functions $P_n^m(x)$ are called associated Legendre functions, and are a
 120 set of orthogonal polynomials widely used in quantum mechanics [53] and
 121 many other fields. If the function $r(\theta, \varphi)$ is known, the coefficients c_n^m can be
 122 calculated as

$$c_n^m = \int_0^{2\pi} \int_0^\pi \sin(\theta) r(\theta, \varphi) Y_n^{m*} d\theta d\varphi \quad (3)$$

123 where the asterisk denotes the complex conjugate. Simple geometrical shapes
 124 such as ellipsoids, cubes, etc. can be obtained by choosing a suitable set of
 125 coefficients [54], with a level of accuracy increasing with N .

126 Using well-known properties of spherical harmonic functions [53], it is
 127 possible to write the representation in Eq. (1) in a different form which uses
 128 real rather than complex-valued functions and coefficients:

$$r_{SH}(N, \theta, \varphi) = a_0^0 Y_0^0 + \sum_{n=1}^N \left[a_n^0 Y_n^0 + \sum_{m=1}^n P_n^m(\cos \theta) (a_n^m \cos(m\varphi) + b_n^m \sin(m\varphi)) \right] \quad (4)$$

129 where $Y_0^0 = \sqrt{\frac{1}{4\pi}}$. The set of coefficients $\{a_n^m\}$ and $\{b_n^m\}$ carry all the infor-
 130 mation on the particle shape.

131 Laser scanning and computed tomography are increasingly widely used
 132 to obtain the point cloud of a particle's surface and study the morphology
 133 characteristics of different particles in nature [55]. After converting the 3D
 134 point cloud data into polar coordinates, established techniques can be used
 135 to extract the set of coefficients of a spherical harmonic expansion [54, 56].

136 If the surfaces of a large number of particles are extracted from a par-
 137 ticular sample, the statistics (or population) of coefficients $\{a_n^m\}$ and $\{b_n^m\}$
 138 represent the 'fingerprint' of that particular sample or set of particles [56].
 139 Once the distribution of coefficients is known, sets of coefficients can be

Figure 1: Particle representations with maximum degrees $N=0, 8, 20$ and 100 . The coefficients $\{a_n^m\}$ and $\{b_n^m\}$ have been generated from uniform distributions

generated easily, allowing the simulation of a sample which is statistically identical to the experimental one.

Fig. 1 shows four representations obtained by truncating the expansion at $N=0, 8, 20$ and 100 . Here the coefficients $\{a_n^m\}$ and $\{b_n^m\}$ have been obtained from a uniform distribution in the interval $[-0.2, 0.8]$. As N increases, the particle shape becomes more and more refined. The high-degree terms of the expansion are mainly responsible for microscopic details of the shape, e.g., the surface roughness.

Figure 2: a) Contact detection between one single point and a sphere; b) Contact detection between a point and a particle of any ‘star-like’ shape. In this case a mathematical description of the shape is needed, i.e., $r = r(\theta, \varphi)$

148 3. Incorporation of spherical harmonics into DEM

149 3.1. Contact detection between arbitrary shapes

150 Contact detection between one single point and a sphere involves calcu-
 151 lating the distance d between the point and the sphere’s centre. Contact
 152 implies the function $d - r \leq 0$, where r is the sphere radius. A touching con-
 153 tact corresponds to $d = r$. The same idea can be generalised to particles of
 154 any shape as $d - r(\theta, \varphi) \leq 0$, where θ and φ are the polar angles as shown in
 155 Fig. 2. In this case we need a mathematical description of the shape where
 156 the radius $r(\theta, \varphi)$ changes as a function of θ and φ , namely the spherical
 157 harmonic representation of particle shape introduced in Section 2.

158 Spherical harmonics have the major benefit of providing not only one but
 159 a set of mathematical approximations of a particle's shape, which become
 160 increasingly refined as the degree of the expansion increases. This inherent
 161 property of spherical harmonics is well-suited to a multi-level representation,
 162 raising the question of why spherical harmonics have not previously been
 163 used for contact detection in DEM. The reason is illustrated in Fig. 3. The
 164 standard spherical harmonic representation of a particle does not require the
 165 shape obtained from an expansion to degree N to bound the shape obtained
 166 from a higher expansion to degree $N + j$. Thus, even though the spherical
 167 representation ($N=0$) of an irregularly shaped particle may have no inter-
 168 particle contacts, there is no assurance that a contact would not appear at
 169 $N=5$, for example. The resolution of this problem, so that low-degree expan-
 170 sions bound higher-degree expansions as required for a hierarchical contact
 171 detection scheme, is described in Section 3.2.

172 Instead of a single point, contact detection for two potentially contact-
 173 ing, non-spherical particles requires discretisation of one of the particles into
 174 many nodes, i.e., discrete function representation (DFR) [36–38]. Few nodes
 175 are needed when N is low and the surface is smooth; a higher density of
 176 nodes is needed when N is large and the surface texture needs to be de-
 177 scribed. Discretisation of a particle's surface is required only in the vicinity
 178 of potential contacts rather than for the entire particle which reduces the
 179 computational cost. A remaining issue, however, is the identification of a
 180 suitable discretisation method: if standard polar coordinates were used, the
 181 density of nodes would be highly non-uniform and divergent at the poles.
 182 The method adopted for this study to avoid this problem is described in

Figure 3: Comparison between the spherical harmonic expansions to a) $N=1$ and $N=20$; b) $N=8$ and $N=20$. The low-degree expansions $N=1$ and $N=8$ do not bound the higher-degree expansion to $N=20$

183 Section 3.3.

184 3.2. Adaptation for hierarchical contact detection

185 If N is the maximum degree of the expansion, we assume that the rep-
 186 resentation at degree N is the one which has the correct particle volume
 187 and shape. Evidently $L \leq N + 1$ particle representations can be gener-
 188 ated, meaning that $\{q_1, q_2, \dots, q_L\}$ intermediate values are selected from N
 189 with $q_L = N$. For example, if $N=20$ and $L=3$, we can choose $q_1=0$, $q_2=8$,
 190 $q_3=20$, the first representation being the sphere. To ensure that low-degree
 191 expansions bound higher-degree expansions, we multiply the expansion to
 192 degree $K = q_i$ by an extra coefficient, S_K , to obtain the adapted hierarchical

193 representation of the particle

$$r_{SH}^S(K, \theta, \varphi) = S_K \sum_{n=0}^K \sum_{m=-n}^n c_n^m Y_n^m(\theta, \varphi) = S_K r_{SH}(K, \theta, \varphi) \quad (5)$$

where $S_{q_L} = 1$, $S_K = \prod_{j=1}^{L-i} v_{q_{L-j}}$, $v_{q_j} = \max \left\{ \frac{r_{SH}(q_{j+1}, \theta, \varphi)}{r_{SH}(q_j, \theta, \varphi)} \right\}$ is the maximum of the ratio between the two particle representations q_{j+1} and q_j . The coefficient S_K is a scaling factor that changes only the size of the particle representation, leaving all the other properties of the spherical harmonic expansion unchanged. Calculating the v_{q_j} terms is a straightforward procedure as the shape expanded to degree N is usually defined on a grid of points; therefore the expansion to N entails the calculation of $L - 1$ additional coefficients $\{v_{q_1}, v_{q_2}, \dots, v_{q_{L-1}}\}$. Eq. (5) is easily demonstrated from the recursive relation

$$\begin{aligned} r_{SH}(q_L, \theta, \varphi) &\leq v_{q_{L-1}} r_{SH}(q_{L-1}, \theta, \varphi) \leq v_{q_{L-1}} v_{q_{L-2}} r_{SH}(q_{L-2}, \theta, \varphi) \leq \dots \\ &\leq v_{q_{L-1}} v_{q_{L-2}} \dots v_{q_1} r_{SH}(q_1, \theta, \varphi) \end{aligned} \quad (6)$$

194 The multiplication of the representation to degree K by S_K has a ‘*shrink-*
195 *ing*’ effect, when representation are compared from the lowest to the highest
196 degree, as shown in Fig. 4. The rate of change of represented volumes slows
197 as N becomes large (compare Fig. 4c with Fig. 4d). The change of volume
198 depends on the number of representation levels L : the larger L is, the larger
199 the cumulative change. Hence the ‘all-level’ representation with $L = N + 1$
200 shown in Fig. 4 is a worst-case scenario, while, in any practical implemen-
201 tation, $L < N$ will be used. Using fewer representation levels would have a
202 less pronounced effect.

Figure 4: The effect of multiplying the representation to degree K by the scaling factor S_K when all degrees 0 to N are separately considered in the hierarchical representation. It ensures that the representation at degree K bounds the representation at $K + j$

3.3. Uniform density of nodes in discretisation

Consider initially the problem of uniformly distributing points on the surface of a sphere with radius r . One way to achieve this is to fix the distance between neighbouring points as $d_p = \frac{2\pi r}{N_p}$, with N_p being the number of points on the equator of the sphere. This also fixes the minimum angular distance between points $\Delta\theta = 2\pi/N_p$. Since $l(\theta) = 2\pi r \sin \theta$ is the θ -dependent length of each parallel, a number of points

$$n_p(\theta) = \frac{l(\theta)}{d_p} = N_p \sin \theta \quad (7)$$

Figure 5: a) Uniform distribution of points on the surface of a sphere. The distance between neighbouring points is fixed as $d_p = \frac{2\pi r}{N_p}$, with N_p the number of points on the equator of the sphere. $n_p(\theta)$ points are assigned to each parallel, corresponding to the possible values $\varphi_i(\theta)$ of φ with $i = 1, \dots, n_p(\theta)$. b) Uniform distribution of points on the surface of a non-spherical particle. Additional points (red '+') are added at high surface gradients, where $|r(\theta + \Delta\theta, \varphi + \Delta\varphi) - r(\theta, \varphi)| > d_p$

210 are assigned to each parallel, separated by angular distances $\Delta\varphi(\theta) = 2\pi/n_p(\theta)$.
 211 Once θ has been fixed, the possible values of φ are $\varphi_i(\theta) = \frac{2\pi}{n_p(\theta)}i$ with
 212 $i = 1, \dots, n_p(\theta)$ (see Fig. 5a). This representation solves the problem of di-
 213 vergence at the poles. In fact, the smallest value of θ is $\Delta\theta = 2\pi/N_p$ so from
 214 Eq. (7) $n_p(\Delta\theta) = N_p \sin(\Delta\theta) \sim N_p \Delta\theta = 2\pi$.

215 This uniform discretisation procedure allows nodes to be uniformly dis-
 216 tributed on the surface of a sphere [39]. However, in the case of non-
 217 spherical particles, regions with high surface gradients, where $|r(\theta + \Delta\theta, \varphi +$
 218 $\Delta\varphi) - r(\theta, \varphi)| > d_p$, must be taken into account. This is done by firstly

219 checking the distance between neighbouring points on the same parallel
 220 (θ fixed) of the uniform discretisation and then dividing by d_p , namely
 221 $\text{NINT}(|r(\theta, \varphi_i(\theta) + \Delta\varphi(\theta)) - r(\theta, \varphi_i(\theta))|/d_p) = p$, where NINT stands for
 222 ‘nearest integer’. p points are then added to the uniform representation, cal-
 223 culating $\{r(\theta, \varphi_i(\theta) + d\varphi_p), r(\theta, \varphi_i(\theta) + 2d\varphi_p), \dots, r(\theta, \varphi_i(\theta) + pd\varphi_p)\}$ where
 224 $d\varphi_p = \Delta\varphi(\theta)/p$ (see the ‘+’ symbols indicated in Fig. 5b). The same proce-
 225 dure is followed for neighbouring points on different parallels by changing θ .
 226 However, discretised values of φ on different parallels can be different, i.e.,
 227 $\varphi_i(\theta) \neq \varphi_j(\theta + \Delta\theta)$, $\forall j \in \{1, \dots, n_p(\theta + \Delta\theta)\}$ (see Fig. 5a). Therefore, we need
 228 to find the value $\varphi_j(\theta + \Delta\theta)$ closest to $\varphi_i(\theta)$, namely $\min(|\varphi_i(\theta) - \varphi_j(\theta + \Delta\theta)|)$.
 229 Considering that $\varphi_i(\theta) = i \frac{2\pi}{n_p(\theta)}$ and $\varphi_j(\theta + \Delta\theta) = j \frac{2\pi}{n_p(\theta + \Delta\theta)}$, we get the simple
 230 relation

$$j = \text{NINT} \left(i \frac{n_p(\theta + \Delta\theta)}{n_p(\theta)} \right) \quad (8)$$

231 We therefore calculate $\text{NINT}(|r(\theta + \Delta\theta, \varphi_j(\theta + \Delta\theta)) - r(\theta, \varphi_i(\theta))|/d_p) = p$,
 232 and add the points $\{r(\theta + d\theta_p, \varphi_i(\theta) + d\varphi_p), r(\theta + 2d\theta_p, \varphi_i(\theta) + 2d\varphi_p), \dots, r(\theta +$
 233 $pd\theta_p, \varphi_i(\theta) + pd\varphi_p)\}$, where $d\theta_p = \Delta\theta/p$ and $d\varphi_p = (\varphi_j(\theta + \Delta\theta) - \varphi_i(\theta))/p$.
 234 In this way the representation shown in Fig. 6 is obtained.

235 **4. Case study: two-level representation of two interacting particles**

236 A proof-of-concept code was developed for two interacting particles, rep-
 237 resented at two hierarchical levels of detail, i.e. $L = 2$ with $q_2 = N = 20$
 238 and $q_1 = 8$. These two representations have been arbitrarily chosen for the
 239 purpose of this demonstration whose scope was not to test the dynamics but
 240 to check that this new method is viable and can be easily implemented in a
 241 standard rigid-body dynamics scheme.

Figure 6: Uniform distribution of points on the surface of a non-spherical particle, obtained through the described algorithm

242 To initialise the system, two sets of coefficients were generated from a
 243 uniform distribution: $\{a_{n,1}^m, b_{n,1}^m\}$ for particle 1 and $\{a_{n,2}^m, b_{n,2}^m\}$ for particle
 244 2. From Eq. (4), four representations $r_{SH,i}(q_j, \theta, \varphi)$ were obtained with par-
 245 ticle indices $i=1, 2$ and representation indices $j=1, 2$ ($q_2=20$ and $q_1=8$).
 246 The representations were discretised uniformly as explained in Section 3.3,
 247 and coefficients $S_{8,i}$ were calculated (Eq. (5)), ensuring that $r_{SH,i}(20, \theta, \varphi) \leq$
 248 $S_{8,i} r_{SH,i}(8, \theta, \varphi) = r_{SH,i}^S(8, \theta, \varphi)$. Here we reserve the word ‘nodes’ to refer
 249 to those points which discretise $r_{SH,i}^S(8, \theta, \varphi)$, and ‘asperities’ for the points

250 discretising $r_{SH,i}(20, \theta, \varphi)$. On Fig. 7, the former are shown as large blue cir-
 251 cular markers of which there are $m_1^n=164$ nodes for particle 1 and $m_2^n=155$
 252 nodes for particle 2; the latter as small red circular markers with $m_1^a=1800$
 253 and $m_2^a=1900$ asperities for particles 1 and 2, respectively. Fig. 7 shows that
 254 $r_{SH,i}^S(8, \theta, \varphi)$ does not describe the fine features of the particle: it is a bound-
 255 ing shape to be used for contact detection. Hence the numbers of nodes m_i^n
 256 are more than one order of magnitude smaller than the numbers of asperities
 257 m_i^a needed to accurately describe the particles' morphology [57]. The mo-
 258 ments of inertia $\mathbf{I}_i$ were calculated in advance for the $N=20$ representations of
 259 these two particles, assuming a uniform mass density of the objects. For this
 260 proof-of-concept, the m_i^n node positions, coefficients $\{a_{n,1}^m, b_{n,1}^m\}$, $\{a_{n,2}^m, b_{n,2}^m\}$
 261 and $S_{8,i}$ were stored at the start of the simulation.

262 Several important differences between this two-particle demonstration
 263 and a future implementation in a large-scale code, e.g. LAMMPS (see Sec-
 264 tion 6) should be emphasised:

- 265 • In practice, one would always choose to begin with the representation to
 266 degree $q_1=0$, rather than $q_1=8$ in this instance, to take advantage of the
 267 computational efficiency afforded by bounding spheres. In that case,
 268 the first stage of contact detection (sphere–sphere) would proceed as in
 269 a conventional sphere-based DEM code, i.e., neither bounding sphere
 270 would be discretised. This would substantially reduce the number of
 271 potential interparticle contacts before progressing to $q_j > 0$ which is
 272 more computationally costly.
- 273 • In this test case, both particles were discretised in order to calculate
 274 the interparticle force using a Lennard-Jones molecular interaction. In

Figure 7: Two-level representation of two approaching particles $r_{SH,i}^S(8, \theta, \varphi)$ and $r_{SH,i}(20, \theta, \varphi)$, with degrees $q_1 = 8$ and $q_2 = N = 20$, respectively. Blue nodes are used to discretise $r_{SH,i}^S(8, \theta, \varphi)$; red asperities discretise $r_{SH,i}(20, \theta, \varphi)$

DEM, it is usual to adopt a contact law based on Hookean or Hertzian mechanics, in which case only one of two contacting particles would require discretisation while the other would remain as an analytical expression. Furthermore, discretisation is only required in the vicinity of a possible contact. If starting at $q_1=0$, nodes would only be required wherever bounding spheres intersect.

Contact detection employing one discretised particle representation and one analytical representation has previously been discussed in the literature [36,

39]. In order to check whether any of the m_2^n nodes of particle 2 overlap with particle 1, the nodes are parsed to search for overlaps as $d - r_{SH,1}^S(8, \Theta_1, \Phi_1) \leq 0$ where d is the length of the line segment joining the origin of particle 1 and a node of particle 2 (see Fig. 7) and Θ_1 and Φ_1 are the polar angles of the line segment in particle 1's reference frame.

In principle, it would be equivalent to reverse the roles of particles 1 and 2, i.e., use the m_1^n nodes of particle 1 and the analytical representation of particle 2. However, in practice, asperities would not be generated at identical positions if 1 and 2's roles were reversed so there would be a small discrepancy between the computed forces. This disparity would be reduced by increasing the density of nodes describing the discretised surface.

If an overlap is found, the discretised particle's representation is refined around the overlapping nodes. To refine to $N=20$ for this demonstration, the representations $r_{SH,i}(20, \Theta_i \pm \Delta\Theta, \Phi_i \pm \Delta\Phi)$ were used to generate asperities 'on the fly' solely around the Θ_i and Φ_i angles, where Θ_2 and Φ_2 are the polar angles of the line segment joining the origin of particle 2 and the overlapping node of particle 2. Here $\Delta\Theta = |\frac{\Theta_{i+1} - \Theta_i}{2}|$ and $\Delta\Phi = |\frac{\Phi_{i+1} - \Phi_i}{2}|$ stand for the angular half-distance between the overlapping node and the adjacent nodes. The asperities are shown on Fig. 7 for the entirety of both particles rather than for a small region of one particle. Ultimately, once the asperities have been generated where required, the net force is calculated as the sum of the forces from each individual asperity.

It is noted that DEM contact laws for non-spherical particles are lacking at present; additional research in this area is ongoing which will complement the development presented in this paper. These contact laws should involve

the calculation of the normal to the analytical representation, and estimation of the contact width or overlap volume [58]. To calculate the force at the single-asperity level, it would be necessary to assign a portion of the total overlapping volume to each asperity [58].

From forces on the asperities, the torque $\boldsymbol{\tau}_i$ is calculated for each particle and the angular momentum $\mathbf{L}_i$ is updated. However, the moment of inertia, $\mathbf{I}_i$, is time-varying in a global coordinate system. Thus, a suitable body particle-fixed coordinate system is usually introduced, where the inertia tensor $\mathbf{I}_i^B$ contains only non-zero entries on its diagonal, referred to as the principal moments of inertia. By using the rotation matrix, $\mathbf{R}_i$, transforming vectors between the two reference frames, the angular velocity, $\boldsymbol{\omega}_i$, can be calculated as

$$\boldsymbol{\omega}_i = \mathbf{R}_i \boldsymbol{\omega}_i^B = \mathbf{R}_i (\mathbf{I}_i^B)^{-1} \mathbf{R}_i^T \mathbf{L}_i \quad (9)$$

where $\mathbf{R}_i^T$ is the transpose of the $\mathbf{R}_i$ matrix and the relations $\boldsymbol{\omega}_i^B = (\mathbf{I}_i^B)^{-1} \mathbf{L}_i^B$, $\mathbf{L}_i^B = \mathbf{R}_i^T \mathbf{L}_i$ are applied. The rotation matrix $\mathbf{R}_i$ is updated at each time-step by using the standard quaternion approach [59]. The particle rotations and orientation are tracked during the simulation using standard algorithms for rigid-body dynamics.

Fig. 8 shows a snapshot of the two-particle simulation once the particles had come into contact. The small red markers on Fig. 8 denote the asperities generated once the overlap had been detected using the procedure outlined above.

Figure 8: Snapshot of the simulation. The red dots indicate the asperities around overlapping nodes. The smaller black dots indicate the precise morphologies of both particles

329 5. Extension to include particle abrasion by chipping

330 The loss of particle mass is due to three mechanisms: frictional abra-
 331 sion, chipping, and fragmentation. Frictional abrasion during contact sliding
 332 smooths the faces and leads to the formation of flat or cylindrical particles
 333 [60]. Chipping occurs at larger energies, when collisions form shallow cracks
 334 that lead to the production of much smaller fragments [61]. Chipping prefer-
 335 entially attacks the edges and corners of the grains, leading to rounding and
 336 the evolution of particles towards a spherical shape [14, 61]. At sufficiently
 337 large collision energies, fractures propagate throughout a particle and lead

338 to its breakup by fragmentation [62, 63].

339 The spherical harmonic framework, which includes a hierarchy of related
 340 particle shapes, could potentially be applied to capture abrasion of a parti-
 341 cle’s surface by chipping. If the particle is assumed to be bombarded isotrop-
 342 ically by a field of large, rough objects, this would lead to a smoothing and
 343 loss of roughness. In such a case, the normal erosion rate, ds/dt , at which a
 344 region of the surface near a point P erodes depends on the curvature [13]:

$$\frac{ds}{dt} = v(1 + AH + BK) \quad (10)$$

345 where v is a constant, and H and K are the mean and Gaussian curvatures.
 346 The parameters A and B depend on the size of impacting particles, repre-
 347 senting their average (or effective) radius and area, respectively. As expected,
 348 the erosion rate is highest where the curvature is greatest and angular regions
 349 erode much faster than flat ones [64].

350 By considering the particle shape at time t , $r(\theta, \varphi, t) = a(t)(1 + \epsilon(\theta, \varphi, t))$
 351 as a perturbed sphere of radius $a(t)$ and expanding ϵ as a sum of spherical
 352 harmonics,

$$\epsilon(\theta, \varphi, t) = \sum_{n=0}^{\infty} \sum_{m=-n}^n \epsilon_n^m(t) Y_n^m(\theta, \varphi) \quad (11)$$

353 it can be shown that higher harmonics decay with time much more rapidly
 354 than the lower ones [13] and the ellipsoidal one, $n = 2$, lasts the longest.
 355 These mathematical considerations, together with recent experimental re-
 356 sults [12], strongly support the idea that higher harmonics, corresponding to
 357 the surface texture, are the first to be eroded, while ellipsoidal shapes, found
 358 in abundance in nature, take much longer to become spherical, i.e., the sphere
 359 is the equilibrium shape [13]. Therefore, representing the abrasion process

360 through the sequential removal of the highest spherical harmonics is an at-
361 tractive idea. During abrasion, mass is lost and it must be ensured that the
362 high-degree spherical harmonic expansion, representing the original shape,
363 bounds the expansion at any lower degree: the abraded shape. We propose
364 a strategy similar to the one in Eq. (5), multiplying the expansion to degree
365 K by a scaling factor, s_K ,

$$r_{SH}^s(K, \theta, \varphi) = s_K \sum_{n=0}^K \sum_{m=-n}^n c_n^m Y_n^m(\theta, \varphi) = s_K r_{SH}(K, \theta, \varphi) \quad (12)$$

366 where N is the maximum degree, $s_N = 1$, $s_K = \prod_{j=1}^{N-K} 1/u_{N-j}$ and $u_i =$
367 $\max \left\{ \frac{r_{SH}(i, \theta, \varphi)}{r_{SH}(i+1, \theta, \varphi)} \right\}$. Fig. 9 shows a set of four expansions with $N = 40$ and
368 $K=40, 30, 10, 2$ obtained by eliminating higher harmonic terms from the
369 expansion and multiplying by the scaling factor s_K . The removal of the
370 highest harmonics leaves the overall shape unchanged (compare $K=40$ with
371 $K=30$), affecting mostly the particle texture and roughness. However, when
372 the expansion is limited to the lowest harmonics, the particle shape is strongly
373 affected, reducing eventually to an ellipsoid.

374 It has been demonstrated that the mass of particles (M) undergoing a
375 wearing process decreases exponentially with time [12] or distance (x) trav-
376 elled [65] according to

$$M = M_0 e^{-kx} \quad (13)$$

377 where M_0 is initial mass and k is an empirically determined coefficient which
378 depends on the material properties and wearing conditions. Eq. (13) is quite
379 general and has been proven in many different experimental situations [66,
380 67]: it states that while the rate of mass loss due to abrasion is very rapid
381 initially, it slows down with the distance travelled. From Eq. (12), we can

Figure 9: Four expansions for $K=40, 30, 10$ and 2 obtained by eliminating higher harmonic terms from the expansion and multiplying by the scaling factor s_K

382 write the abraded shapes to degree K in spherical coordinates and therefore
 383 calculate their K -dependent volumes as:

$$V_K = \int_0^\pi \int_0^{2\pi} \int_0^{r(K,\theta,\varphi)} \rho^2 \sin(\theta) d\theta d\varphi d\rho = \int_0^\pi \sin(\theta) d\theta \int_0^{2\pi} \frac{r^3(K, \theta, \varphi)}{3} d\varphi \quad (14)$$

384 where $dv = \rho^2 \sin(\theta) d\theta d\varphi d\rho$ is the volume element and $r(K, \theta, \varphi)$ is a shorter

notation to indicate $r_{SH}^s(K, \theta, \varphi)$ in Eq. (12). Fig. 10 shows that the particle volume is a decreasing function of the degree. If the ‘mass-loss’ function is known for a particular process and the density of the particle is constant throughout, the distance x travelled can be estimated from the particle mass M by inverting Eq. (13).

As high harmonics only change the texture of a particle’s surface [12], we would expect a small volume change at a high degree, as reported in literature [51]. However, to ensure that the expansion at higher degrees bound those at lower degrees, we ‘shrink’ the shape using the coefficients s_K . The relative volume change $V_K^r = (V_K - V_{K-1})/V_{ave}$ can be defined where $V_{ave} = \frac{V_K + V_{K-1}}{2}$ is the average volume. V_K^r is plotted as a function of the degree in Fig. 10b. V_K^r shows minor variations at high harmonics, with a growing trend toward low harmonics, as expected.

The change of volume determines the quantity of fines produced. The change of particle surface area is also important as this affects, for example, the particle’s effectiveness as a catalyst (noting that particles are taken to be solid rather than porous which would usually be the case). The area can be estimated by integrating the differential surface area element $dA = |\frac{d\vec{r}}{d\theta} \times \frac{d\vec{r}}{d\varphi}| d\theta d\varphi$, representing the area of each small ‘tile’ in Fig. 9, over θ and φ . $\vec{r}$ is the vector with norm $r(K, \theta, \varphi)$ and direction given by (θ, φ) . It can be shown that $dA = r (r_\varphi^2 + r_\theta^2 \sin^2 \theta + r^2 \sin^2 \theta)^{1/2} d\theta d\varphi$ with $r_\varphi = \frac{d\vec{r}}{d\varphi}$, $r_\theta = \frac{d\vec{r}}{d\theta}$, so that the surface area, A_K , to degree K is

$$A_K = \int_0^\pi \int_0^{2\pi} r^2(N, \theta, \varphi) (r_\varphi^2 + r_\theta^2 \sin^2 \theta + r^2(N, \theta, \varphi) \sin^2 \theta)^{1/2} d\theta d\varphi \quad (15)$$

The behaviour of A_K as a function of degree is reported in Fig. 11a. As for the volume V_K , the decrease of area is due to the shrinking of the shape, so

Figure 10: Particle volume V_K and relative volume change V_K^r as a function of the degree. Red circles refer to the expansions shown in Fig. 9

the relative area change, $A_K^r = (A_K - A_{K-1})/A_{ave}$, is also shown (Fig. 11b),
 where $A_{ave} = \frac{A_K + A_{K-1}}{2}$ is the average area. A_K^r changes more significantly
 as the degree is reduced, particularly at lower degrees.

6. Discussion and proposed implementation

Sections 3–5 establish the fundamental principles of a new method for
 the simulation of abradable, irregularly shaped particles. Next this will be

Figure 11: Particle area A_K and relative area change A_K^r as a function of the degree

415 implemented in a suitable code, e.g. LAMMPS [50]. Through a suitable
 416 choice of representations, particles will be simulated at multiple levels of
 417 resolution, beginning with bounding spheres ($N=0$) before progressively re-
 418 fining the shapes around potential contacts to ultimately achieve the desired
 419 level of shape fidelity at the interparticle contacts. The fidelity can change
 420 temporally, e.g., particles may be simulated less accurately during sample

421 preparation than subsequently. The fidelity could also depend on the loca-
 422 tion of a particle within the simulation domain, i.e., more refined particles
 423 (higher N) could be used at locations within the domain which are deemed to
 424 be of particular interest. This raises the possibility of emulating the common
 425 practice in finite element analyses of simulating regions within the domain
 426 with greater refinement (smaller elements) than others, e.g., at the boundary
 427 of the domain. The commonly used sphere-based contact detection algorithm
 428 can be retained for the bounding spheres. The intention is to carry out the
 429 hierarchical refinement of the particles within the contact law (e.g., ‘pair
 430 style’ in LAMMPS).

431 There is, of course, considerable potential to improve the computational
 432 performance of this method compared to the two-particle demonstration.
 433 For example, no information about computed overlaps or nodes is carried
 434 forward to the following time step which has the potential to reduce the
 435 computational effort substantially. In addition, a high density of nodes has
 436 been used for discretisation in this two-particle demonstration. An open
 437 question, which will be investigated as part of the future work on developing
 438 this method, is the optimal density of nodes to strike an appropriate balance
 439 between efficiency of contact resolution and accuracy. This density of nodes
 440 should change between representations: the higher the degree, the greater
 441 the density of nodes needed to describe shape details and surface texture.
 442 Reducing the number of nodes without significantly degrading the accuracy
 443 could greatly reduce the computational cost.

444 A physical rationale, e.g., Archard’s law, will be imposed for particle

445 abrasion:

$$Q = WF_n l_t \quad (16)$$

446 where Q is the volume of material removed, W is a constant, F_n the normal
447 load and l_t the sliding distance. Since F_n and l_t are known quantities for
448 each pair of interparticle contacts in DEM, Q can be calculated once W
449 has been calibrated appropriately using experimental data. Therefore, from
450 the number of collisions, it will be possible to estimate the loss of volume
451 and then the particle shrinkage to a lower degree K ; this latter representation
452 will become the new reference shape for the hierarchical representation. More
453 precisely, each particle representation, $r_{SH}^S(a, h, \theta, \varphi)$, will be characterised by
454 two parameters, a and h , representing ‘abrasion’ and ‘hierarchical’ indices,
455 respectively. The values of a and h constitute a two-dimensional array, as
456 each abraded shape will correspond to a number of possible representations.

457 7. Conclusions

458 In this paper, we have presented the essential foundation for incorporat-
459 ing spherical harmonics into a DEM simulation for the purpose of simulating
460 the dynamics of realistically shaped particles. We have shown that spher-
461 ical harmonics can be used not only for the representation of particles via
462 the calculation of the coefficients, but could be practically integrated into a
463 DEM code and even benefit contact detection between non-spherical particles
464 through the use of suitable scaling factors. A detailed description of particle
465 shape is computed only at interparticle contacts which reduces the computa-
466 tional cost, while the use of the scaling factors enables a hierarchical contact
467 detection approach. This paves the way for the widespread use of spherical

468 harmonics in DEM simulations. The feasibility of a spherical harmonic-based
469 DEM simulation has been shown for only two particles, where a simple al-
470 gorithm for the generation of asperities ‘on the fly’ is added to a classical
471 rigid-body dynamics scheme.

472 Additionally, based on mathematical considerations and experimental ev-
473 idence, it has been shown that abrasion can be simulated by the sequential
474 removal of high harmonics from the spherical harmonic expansion. This
475 abrasion can be related to a microscopic wearing law, such as Archard’s law,
476 and incorporated into the hierarchical particle simulation approach. Each
477 abraded shape will be associated with a set of multi-level shape representa-
478 tions, i.e., spherical harmonic coefficients.

479 Potential improvements and future development will include the calcula-
480 tion of an *optimal* density of nodes, to reduce the computational cost without
481 significantly degrading the accuracy.

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